

# THE ANALYTIC LANCZOS METHOD

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The classical formalism of the Moment Problem has been combined with a cumulant approach and applied to the extensive many-body problem. This has yielded many new exact results for many-body systems in the thermodynamic limit - for the ground state energy, for excited state gaps, and for arbitrary ground state averages. The method applies to any extensive Hamiltonian system, for any phase or symmetry arising in the model, whether on a lattice or in the continuum, and for any dimensionality. The theorems are of a nonperturbative nature with respect to any couplings occurring in the model.

## 1 The Early Development of the Lanczos Algorithm

The Lanczos algorithm or method has been of interest to physicists because it is an essentially non-perturbative approach to physical problems with strong coupling, such as occur in the extensive many-body systems of condensed matter physics. In this method the Hamiltonian is used to generate a sequence of orthonormal states  $\{|\psi_n\rangle\}_{n=1,2,\dots}$  and Lanczos coefficients  $\{\alpha_n\}_{n=0,1,\dots}, \{\beta_n\}_{n=1,2,\dots}$ , from a suitably chosen trial state  $|\psi_0\rangle$  through the following recurrence

$$|\psi_{n+1}\rangle = \frac{1}{\beta_{n+1}}[(\hat{H} - \alpha_n)|\psi_n\rangle - \beta_n|\psi_{n-1}\rangle], \quad (1)$$

so that the Hamiltonian in this new basis is tridiagonal

$$T_n = \begin{pmatrix} \alpha_0 & \beta_1 & & & \\ \beta_1 & \alpha_1 & \beta_2 & & \\ & \beta_2 & \ddots & \ddots & \\ & & \ddots & \ddots & \beta_n \\ & & & \beta_n & \alpha_n \end{pmatrix}. \quad (2)$$

In the mathematical and statistical arena the Lanczos Process has been long understood as one manifestation of a body of intimately connected mathematical subjects, namely - the Moment Problem<sup>1,2</sup>, Orthogonal Polynomial Systems<sup>1,2</sup>, Pade Approximations<sup>3,4</sup>, Analytic Continued Fraction Theory<sup>5,6</sup> and Krylov Subspace Methods<sup>7</sup>. One such equivalence is that the Lanczos process applied up to  $n_T$  iterations to generate the Lanczos coefficients  $\{\alpha_n\}_{n=0}^{n_T}, \{\beta_n\}_{n=1}^{n_T}$  is precisely equivalent to generating the first  $2n_T + 1$  moments  $\{\mu_n\}_{n=0}^{2n_T+1}$  defined by  $\mu_n \equiv \langle \hat{H}^n \rangle$  ( $\langle \hat{O} \rangle$  denotes the expectation value with respect to the trial state).

The traditional use of the Lanczos algorithm has been in a purely numerical way, that is to say as a numerical technique for exact diagonalisation of very large matrices that arise in treating many-body problems in small finite systems<sup>8</sup>, or in the treatment of the one-electron problem in disordered or aperiodic systems,

as in the Recursion Method of Haydock<sup>9</sup>. The potential of taking the Lanczos algorithm far beyond these limitations, into a more powerful, universal formalism has not been widely appreciated, although some inkling of this was apparent in the suggestion of Mattis<sup>10</sup> concerning the exact mapping of the many-body problem onto a one-dimensional nearest-neighbour model. This idea was explored in some applications to the Kondo and Wolff models by Mancini and Mattis<sup>11,12,13</sup>. We wish to emphasize to the reader that our approach here is quite different from that used in the exact diagonalisation studies of finite systems in two respects - we do not construct a full basis for a finite system but manipulate basis vectors and coefficients of an arbitrarily large system analytically and symbolically, and we perform every iteration exactly and therefore need not concern ourselves with round-off or loss of orthogonality issues.

While little use or development of the mathematical constructs were employed in exact diagonalisation methods, some of the ideas were used in other formalisms. Formalisms were developed under the name of the Recursion Method<sup>9,14,15,16</sup> or related methods<sup>17,18,19</sup> for one-electron problems, but in the last analysis every calculation was a numerical evaluation, i.e. explicit construction of the orthogonal polynomials via 3-term recurrences and then the continued fraction representation of the density of states. Some questions were raised concerning the generalisation to genuine many-body problems<sup>20</sup> but this was not realised at the time. Other formalisms, treating many-body systems and stochastic processes in the thermodynamic limit, which arose from this mathematical legacy were the Memory Function formalism<sup>21,22,23,24,25</sup>, the Recursion Method<sup>26</sup> (not to be confused with the previous use of the same term) and the Projection Method<sup>27,28,29,30,31</sup>. However all these methods were applied only formally, that is to say the consequences of introducing these tools into the many-body problem was not systematically followed through or explored - the recursion process would be carried out up to a finite number of steps and truncated in an ad-hoc manner. This can be done analytically by hand for the first few steps, but usually higher steps are calculated on a computer by constructing an equivalent graphical description of the problem and making the combinatorial evaluations that arise. The formalisms are precise and exact in this regard but being truncated in this manner they have not converged  $n_T \rightarrow \infty$ . This is a serious issue because while  $n_T$  may be numerically large, say 20 or 30, one also wants to follow this Lanczos convergence with the thermodynamic limit  $N \rightarrow \infty$ , but the problem is that the value of  $n_{opt}$ , to assure convergence to a given accuracy, will scale with  $N$  at best, and may sometimes scale with a higher dependence.

## 2 The New Developments

However it is possible to transcend these limitations in the process of constructing the mathematical formalism properly embedded in its physical context. The first key ingredient is to find a way of incorporating the system size scaling for the extensive system into the existing formalism from the outset. The solution to this is obvious - describe everything in terms of cumulants, connected moments or semi-invariants<sup>32</sup>  $\{\nu_n\}_{n=1}^{\infty}$  ( $\nu_n \equiv \langle \hat{H}^n \rangle_c$ ) instead of moments. The defining relationship

is

$$\langle e^{t\hat{H}} \rangle = \sum_{n=0}^{\infty} \mu_n \frac{t^n}{n!} \equiv \exp \left( \sum_{n=1}^{\infty} \nu_n \frac{t^n}{n!} \right), \quad (3)$$

and there exists a unique transformation between the set of first  $n_T$  cumulants and the set of first  $n_T$  moments. Cumulants scale with the system size in the following way

$$\nu_n = c_n N, \quad \nu_n = c_n N + m_n, \quad (4)$$

in the ground state sector and other sectors respectively, ignoring boundary conditions. The coefficients  $c_n$ ,  $m_n$  are independent of  $N$  and functions of coupling constants and other parameters in the trial state. With this scaling form all information regarding finite-size scaling is lost, but it is the simplest approach. Unconnected moments encapsulate the information about a system in a very redundant way and which leads to problems of ill-conditioning.

Once the above step is taken then many results become quickly apparent. The first result arises from the substitution of the cumulant Eq. (4) into the explicit expression for the moments, and then into the Lanczos coefficients, and expanding the resulting forms in a large  $N$  expansion - and the result is a remarkably simple and perfectly universal expansion - the “Plaquette Expansion”<sup>33,34,35</sup> - as a function of an arbitrary Lanczos iteration number  $n$

$$\frac{\alpha_n}{N} = c_1 + n \left[ \frac{c_3}{c_2} \right] \frac{1}{N} + \frac{1}{2} n(n-1) \left[ \frac{3c_3^3 - 4c_2 c_3 c_4 + c_2^2 c_5}{2c_2^4} \right] \frac{1}{N^2} + \dots, \quad (5)$$

and

$$\begin{aligned} \frac{\beta_n^2}{N^2} &= n c_2 \frac{1}{N} + \frac{1}{2} n(n-1) \left[ \frac{c_2 c_4 - c_3^2}{c_2^2} \right] \frac{1}{N^2} \\ &+ \frac{1}{6} n(n-1)(n-2) \left[ \frac{-12c_3^4 + 21c_2 c_3^2 c_4 - 4c_2^2 c_4^2 - 6c_2^2 c_3 c_5 + c_2^3 c_6}{2c_2^5} \right] \frac{1}{N^3} + \dots \end{aligned} \quad (6)$$

It can be shown<sup>36</sup> that just retaining the first terms in each coefficient can be interpreted as a manifestation of the Central Limit Theorem and a description in terms of Gaussian fluctuations, while retaining the first two terms in each describes dynamical processes governed by the Binomial distribution and all related ones. In this way many of the distributions of statistics arise naturally in such an expansion, and in fact simple interacting physical models can be found which are exactly represented by a finite number of terms in this expansion<sup>36</sup>.

It should be noted that in each term of the above the degree of the polynomial in  $n$  is the same as the inverse power of  $N$  so that the following limit  $n, N \rightarrow \infty$  exists at fixed  $s \equiv n/N$ . Although the above is just a Taylor series expansion in  $1/N$  we conjecture that the exact Lanczos coefficients exhibit the following general confluence

$$\alpha_n(N) \xrightarrow{n, N \rightarrow \infty} N \alpha(s), \quad \beta_n^2(N) \xrightarrow{n, N \rightarrow \infty} N^2 \beta^2(s). \quad (7)$$

In the next step if one defines the spectral envelope functions

$$\begin{aligned} e_n(N) &= 1/2 \left\{ \alpha_n + \alpha_{n-1} - \sqrt{(\alpha_n - \alpha_{n-1})^2 + 16\beta_n^2} \right\}, \\ &\xrightarrow{n, N \rightarrow \infty} e(s) = \alpha(s) - 2\beta(s), \end{aligned} \quad (8)$$

then one can employ theorems on bounds to the extremal zeros of Orthogonal Polynomials to arrive at an exact theorem for the ground state energy<sup>37</sup>

$$\epsilon_0 = \inf_s [e(s)] , \quad (9)$$

and if this occurs at a finite point it is denoted  $s_0$ . This result constitutes an exact diagonalisation of the many-body problem in the thermodynamic limit, as the formalism expresses results in terms of the tridiagonal matrix elements, or Lanczos coefficients. From this it is a simple step to finding the ground state average for an arbitrary operator  $\hat{O}$ <sup>38</sup>

$$\langle \hat{O} \rangle = \left[ \delta^O \alpha(s) - \frac{\delta^O \beta^2(s)}{\beta(s)} \right]_{s_0} , \quad (10)$$

where the operator Lanczos coefficients are constructed from the operator cumulants

$$\delta^O \nu_{n+1} = \sum_{k=0}^n \langle \hat{H}^{n-k} \hat{O} \hat{H}^k \rangle_c \rightarrow \delta^O \alpha, \delta^O \beta^2 , \quad (11)$$

in the same manner as the pure Lanczos coefficients. The excited state gap, between the ground state and an excited state in another sector, is just the difference between two ground state energy densities,  $\epsilon_1 - \epsilon_0 = \Delta\epsilon/N$  and is thus<sup>39</sup>

$$\Delta\epsilon = \left[ \delta^G \alpha(s) - \frac{\delta^G \beta^2(s)}{\beta(s)} \right]_{s_0} , \quad (12)$$

where the gap Lanczos coefficients are constructed from the gap cumulants (constructed using a trial state with the excited state quantum numbers)

$$\nu_n = c_n N + \delta^G c_n \rightarrow \delta^G \alpha, \delta^G \beta^2 . \quad (13)$$

For the excited state gap in the same sector, the following peeling theorem holds<sup>40</sup>

$$\Delta\epsilon = 2 \lim_{n, N \rightarrow \infty} N [e(s) - e_n(N)]_{s_0} . \quad (14)$$

In its application to non-integrable models the above expansion, Eq.(5,6), is generated from a finite set of low order cumulants and then truncated at some finite order and the above theorems applied without the need for any extrapolation. Some examples where this has been successfully employed are the 1 and 2-dimensional Heisenberg models<sup>41,38</sup> and lattice gauge models<sup>42,43</sup>. There are also examples of this method used in an essentially exact manner, namely for a 1-dimensional solvable spin model with a phase transition at  $T = 0$ <sup>44</sup>, where the convergence properties of the method have been examined.

### 3 Summary

As we have seen the Analytic Lanczos Method is an important stage in the development of Lanczos methods in the extensive many-body problem. Amongst its virtues

are that is general purpose - it works for any Hamiltonian, lattice or continuum, quantum mechanical or classical, in all dimensions  $D$ , for any phase or symmetry of the model, it is non-perturbative in couplings, it works exactly in the thermodynamic limit  $N \rightarrow \infty$  and it applies to ground state or  $T > 0$  properties. It is accurate and systematic in that there is a development in successive orders so that some control of the errors can be made. It has a flexible implementation in that the treatment can be either analytic, semi-analytic or numerical depending on the degree of integrability of the model at hand, that one is free to choose the trial state, within very general limits relating to the symmetry of the target state, and that one can combine it with other methods, e.g. variational, mean-field, . . . .

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